

Exact diagonalization analysis of the Anderson-Hubbard model and comparison to real-space self-consistent Hartree-Fock solutions

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We have obtained the exact ground state wave functions of the Anderson-Hubbard model for different electron fillings on a 4×4 lattice with periodic boundary conditions. When compared to the uncorrelated ground states (Hubbard interaction set to zero) we have found evidence of very effective screening, producing smaller charge inhomogeneities due to the Hubbard interaction, particularly at 1/2 filling, and have successfully modelled these local charge densities with non-interacting electrons that experience a static screening of the impurity potentials. Further, we have compared such wave functions to self-consistent real-space unrestricted Hartree-Fock solutions and have found that these approximate ground state wave functions are very successful at reproducing the local charge densities, and may indicate the role of dipolar backflow in producing a novel metallic state in two dimensions.

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Many transition metal oxides display phenomena that are believed to be associated with both strong electronic correlations and disorder. Various metal-to-nonmetal transitions,¹ and some properties of the underdoped high-T_c cuprate superconductors^{2,3,4} are examples of such physics. Presently the study of such systems is a very active field of research in condensed matter physics.

Theoretically, the simplest model that hopefully represents some of the key physics of such systems is the so-called Anderson-Hubbard Hamiltonian. The Anderson model⁵ is given by

$$\hat{H}_A = \sum_{i,\sigma} V_i \hat{n}_{i,\sigma} - t \sum_{\langle i,j \rangle, \sigma} (\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + h.c.) \quad (1)$$

where $i, j = 1 \dots N$ denote the sites of the lattice, $\langle i, j \rangle$ implies that i and j are near neighbours, $\hat{c}_{i,\sigma}$ ($\hat{n}_{i,\sigma}$) is the destruction (number) operator for an electron at site i with spin σ , and the hopping energy is denoted by t . The on-site energy at site i is given by V_i , and in this report we have examined a 50/50 binary alloy model, where V_i is set equal to $W/2$ (for an A site) or $-W/2$ (for a B site). The particular complexion of disorder that is used in this study can be seen in Fig. 2 – the filled circles represent the A sites, while the open circles represent the B sites. The electron interactions that are included are represented by the Hubbard term, given by

$$\hat{H}_H = U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} \quad (2)$$

The Anderson-Hubbard model is formed from the sum of \hat{H}_A and \hat{H}_H .

There are two dimensionless energy scales in this problem: W/t and U/t . Due to the challenge of the computational task (see below), in this report we present results for $U/t = 8$ only – such an interaction energy is equal to the bandwidth of the non-interacting ordered systems,

that being $8t$. We have examined the weak to strong disorder regimes using $W/t = 4, 6, 7, 8, 9, 10$ and 12, and have completed calculations for fixed electronic densities of 1/4, 3/8 and 1/2 filling.

In our numerical work we have studied a binary alloy for a 4×4 lattice with periodic boundary conditions, and have included an on-site Hubbard repulsion energy equal to the bandwidth of the ordered, non-interacting problem. Due to the lack of translational periodicity, one must determine all of the 16-choose-8 squared (for 1/2 filling), or roughly 166 million probability amplitudes, and to date there are no exact wave functions available for such a large spatially disordered system. (While work on ordered systems⁶ has indeed studied larger Hilbert spaces, previous work⁷ on this and related (spinless fermion) spatially inhomogeneous Hamiltonians have not surpassed Hilbert spaces of dimension $\sim 3 \times 10^5$, less than 1/500th the size that we have used.) The role of exact diagonalization computational work in the elucidation of the physics of strongly correlated electronic systems is well known – it provides numerically exact solutions that are free from approximations. The only drawback is that relatively small systems must be examined. Larger systems can indeed be studied using quantum Monte Carlo simulations, and have been completed in both two⁸ and three⁹ dimensions. Our data is complementary to such work. Therefore, these results can now be used as benchmarks gauging the success of proposed theories, such as Hartree-Fock, which is discussed below, or the popularly used dynamical mean field theory (DMFT).¹⁰ Some analogous benchmarking comparisons of DMFT for ordered systems have recently been completed.¹¹

For this cluster one can exactly diagonalize the Hamiltonian matrix and find the ground state wave function using the Lanczos algorithm. Besides the energy of these states, we have found the local charge densities as well as one characterization of the magnetic properties given

(a)				
1.755	0.140	0.284	1.825	
0.262	0.189	1.778	1.752	
0.177	1.714	0.173	0.261	
1.842	0.251	1.771	1.827	
(b)				
1.082	0.941	0.906	1.057	
0.919	0.925	1.091	1.080	
0.925	1.105	0.913	0.918	
1.075	0.910	1.094	1.060	
(c)				
1.064	0.959	0.919	1.039	
0.937	0.941	1.079	1.063	
0.941	1.095	0.925	0.935	
1.061	0.922	1.079	1.041	

TABLE I: In (a) the exact local charge densities are listed for the $U/t = 0$ non-interacting ground state at 1/2 filling for $W/t = 4$; (b) shows analogous data, but now for the exact interacting systems with $U/t = 8$; (c) shows the local charge densities for the interacting problem, now calculated within the Hartree-Fock approximation.

by $\mathbf{S}_i \cdot \mathbf{S}_j$ for i and j being nearest neighbours.

The disorder potential without the Hubbard energy is sufficient to produce a strongly inhomogeneous system, even for moderately small disorder. This is demonstrated in part (a) of TABLE I in which we have listed the local charge densities for $W/t = 4$ and $U = 0$. The A sites have charge densities from 0.14 to 0.28, whereas the B sites have local charge densities from 1.71 to 1.84. How effective is the Hubbard interaction energy in screening the disorder potential? For $U/t = 8$ the answer from exact diagonalization is found in part (b) of TABLE I. With the Hubbard interaction the local charge densities for both A and B sites now range from only 0.91 to 1.11, and inspection of the data for the non-interacting and interacting charge densities makes evident the effectiveness of the Hubbard energy in producing a much more

uniform charge density.

However, it is to be emphasized that when one is away from 1/2 filling the homogenization of the local charge densities is far from complete. That is, making the Hubbard energy of the order of or larger than the disorder potential does not necessarily lead to complete screening of the disorder. As an example note that for $U/t = 8$ and $W/t = 4$ for 3/8 filling, one finds a bimodal distribution of the local charge densities peaked at roughly 0.5 (for the A sites) and 1.0 (for the B sites).

One important element of work towards the understanding of such systems is the characterization of electronic screening of the (impurity) disorder potential, and recent publications^{12,13} have stressed the importance of disorder screening in interacting systems. We have examined the simplest variant of such an approach. To be specific, for *non-interacting* electrons we have determined the ground states with screened impurity potentials, *viz.* for effective on-site energies given by

$$V_i \rightarrow V_i^{eff} = \frac{V_i}{\varepsilon} \quad (3)$$

Solving for the local charge densities for such a model, we fit the static dielectric constant, ε , for each filling and W/t by minimizing the mean-squared difference of these densities in comparison to the exact local charge densities. This procedure is quite successful, especially (as expected) at 1/2 filling, and in TABLE II we compare charge densities for $W/t=12$ from which one can see the impressive agreement (note that this is for $U/t = 8$) between these approaches. For this parameter set and filling, we find $\varepsilon \approx 2.6$.

The simplest and most common approach to finding approximate solutions for interacting systems is that of using a self-consistent, real-space unrestricted Hartree-Fock (HF) approach, which previously have been employed in various ways in previous studies^{1,14,15}.

In such a HF approach one ignores terms that are proportional to fluctuations about mean values squared, and thus one approximates the local Hubbard interaction being replaced by (here we ignore the possibility of local superconducting pairing correlations)

$$\begin{aligned} \langle \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} \rangle &= (\bar{n}_{i,\uparrow} + \delta \hat{n}_{i,\uparrow})(\bar{n}_{i,\downarrow} + \delta \hat{n}_{i,\downarrow}) - (h_i^+ + \delta \hat{h}_i^+)(h_i^- + \delta \hat{h}_i^-) \\ &\approx \hat{n}_{i,\uparrow} \bar{n}_{i,\downarrow} + \hat{n}_{i,\downarrow} \bar{n}_{i,\uparrow} - \bar{n}_{i,\uparrow} \bar{n}_{i,\downarrow} - \hat{h}_i^+ h_i^- - \hat{h}_i^- h_i^+ + h_i^+ h_i^- \end{aligned} \quad (4)$$

where the effective local fields h_i^\pm are given by

$$h_i^+ \equiv \langle \hat{S}_i^+ \rangle \quad h_i^- \equiv \langle \hat{S}_i^- \rangle . \quad (5)$$

Then, one must find self consistently the local spin-resolved charge densities and local fields that minimize the variational estimate of the ground state energy.

The HF approach is a variational one in which the lowest energy solution within the product state Hilbert space is found. A comparison of the energies for different fillings and disorder is shown in Fig. 1, and the agreement between the exact and HF energies is seen to improve with increasing disorder, as expected.

(a)				
1.811	0.110	0.219	1.875	
0.193	0.145	1.821	1.813	
0.140	1.775	0.143	0.199	
1.870	0.192	1.819	1.874	
(b)				
1.813	0.106	0.231	1.874	
0.199	0.148	1.816	1.806	
0.141	1.759	0.147	0.199	
1.873	0.199	1.811	1.877	

TABLE II: In (a) the exact local charge densities are given for the $U/t = 8$ interacting ground state at 1/2 filling for $W/t = 12$; (b) shows analogous data, but now for the exact non-interacting system in which the impurity potential $W/t = 12$ is screened as in Eq. (3), for a static, homogeneous dielectric constant of $\varepsilon = 2.6$.

It is common rubric that HF works best for disordered systems (in comparison to ordered systems), but the critiquing of such a belief requires that one be in possession of exact solutions with which one can compare approximate solutions. One such comparison is found in part (c) of TABLE I shows the local charge densities for the HF ground state for $W/t = 4$ and $U/t = 8$ for 1/2 filling (the spins are found to be collinear for this state, so it is permissible to set $h_i = 0$ – see below). Clearly the agreement between the exact and HF ground states is very good – the maximum absolute difference between exact and HF charge densities is 0.019. This quantitative agreement is found to be repeated for all W/t , U/t and electronic fillings. One particular example of the success of this approximation is found for $W/t = 12$, $U/t = 8$ at 1/4 filling – for these parameters the largest absolute difference between the exact and HF local charge densities is only 0.002.

We now turn to what one can learn from the HF solutions concerning the spin degrees of freedom for such systems, both the spin-spin correlations and the spatial arrangement and orientations of the spins. For the HF solutions there is some freedom of choice in specifying the possible effective fields that are allowed. That is, if the h_i^\pm are set to zero then the only nonzero expectation values of $\langle \hat{\mathbf{S}}_i \cdot \hat{e}_\alpha \rangle$, where $\alpha = x, y, z$, are for the z components. Such solutions correspond to (potentially) non-paramagnetic spin arrangements with collinear spins. If the h_i^\pm are allowed to be non-zero but constrained to be real then $h_i^+ = h_i^-$ and both the x and z components can be nonzero. This allows for the possibility of the HF solutions having non-collinear (but still coplanar) spins lying in the xz plane – below we will refer to such solutions as “twisted spin configurations”. Both of these circumstances lead to restricted HF solutions; only when the h_i^\pm are allowed to assume complex values does one have the fully unrestricted solutions. In our numerical

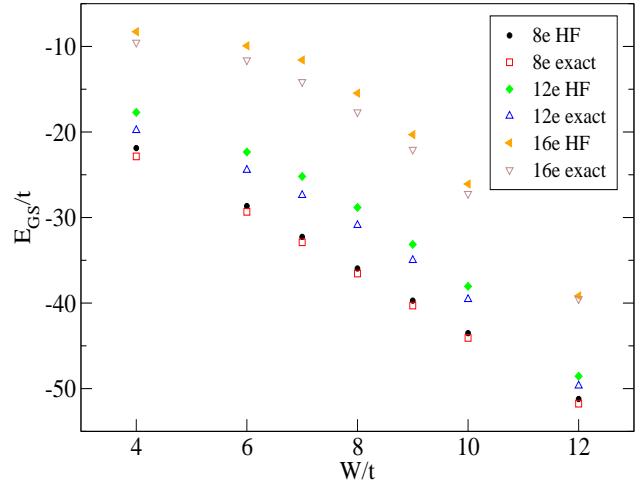


FIG. 1: [Colour online] The exact *vs.* real-space self-consistent Hartree-Fock energies for the binary alloy Hamiltonian discussed in the text. The Hubbard interaction is fixed to be $U/t = 8$, and the lower/middle/upper curves correspond to fixed electronic densities of one-quarter/three-eighths/half filling, namely 8e, 12e and 16e.

work on a 4×4 lattice, we have found that for all system parameters and fillings the HF states correspond to either collinear or coplanar spin configurations.

In contrast to the success of the HF wave functions in producing an excellent approximation for the local charge densities of the exact ground state, since these wave functions are product states the spin degrees of freedom are essentially classical (although the moments on each site can be different than 1/2) and therefore the effectiveness of this approximation in reproducing the spin correlations in the ground state is not expected to be as good. Indeed this is what we find – there is only a reasonable *qualitative* similarity between the exact and HF near-neighbour spin-spin correlations. As one typical example note that for $W/t = 6$ and $U/t = 8$ at 1/2 filling, the average (absolute) difference between the exact and HF evaluations of $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ for i, j being near neighbours is almost 20% – for some near neighbours the HF correlations do not even have the same sign as found in the exact solutions. Further, comparing the exact and HF results using a spatially averaged mean-squared difference, while the local charge densities improve with increasing disorder, similar to the energies of Fig. 1, the spin-spin correlations become increasingly worse with increasing disorder.

The spin degrees of freedom that are present in the HF solutions do contain some potentially important information, and here we mention one possible relationship of our results to other studies. That is, the spin arrangement that we find may have a bearing on a recent proposal for a novel metallic phase in two dimensions.¹⁵ The authors of this paper found that at 1/2 filling and for a disorder strength that was approximately equal to the Hubbard energy there was a significant delocalization of the effective one-electron HF eigenstates at the Fermi energy,

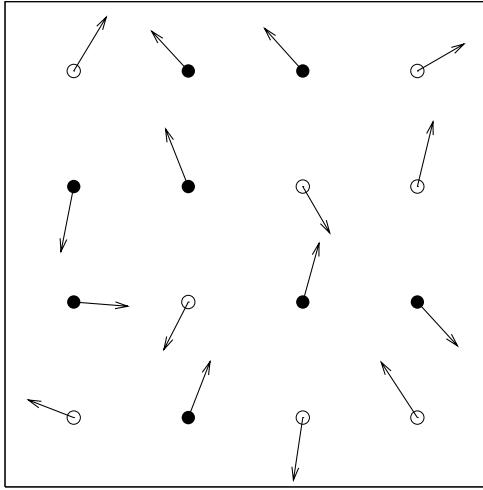


FIG. 2: The spin configuration for a 1/2 filled system with $W/t = 7$ and $U/t = 8$. The filled circles denote A sites and the open circles denote B sites. The length of each vector is proportional to the magnitude of the magnetic moment on that site.

and thereby forecast the existence of a metallic state in two dimensions. An understanding of the physics of this result remains an outstanding problem.

We have found an interesting result in our HF studies that relates to this problem, that being that when we focus on 1/2 filling, only for $W/t = 7$ and 8 (for $U/t = 8$) do we find non-collinear spin configurations; for all other values of W/t we find collinear HF ground states. In Fig. 2 we show the non-collinear spin configuration found for 1/2 filling for $W/t = 7$ and $U/t = 8$. It is in this same parameter regime that these authors¹⁵ found the existence of a novel metallic phase, and the role that these spin configurations may play in such a transition is an interesting question to explore. Further, some evidence

of this physics is also found in a comparison of the exact and HF wave functions. Out of all of the exact wave functions that we obtained, the only (non-singlet) triplet ground state was for 1/2-filling and $W/t = 7$. In fact, for this system the HF state had a net magnetic moment of 1, consistent with the exact ground state.

To answer the question of what, if anything, does the non-collinear spin configuration of the HF solution have to do with the enhanced delocalization of electrons found in Ref. 15, we draw a parallel to the work studying a single hole moving in an antiferromagnet background (described by the $t - J$ model). Speculation of the potential physics behind the metallization in two dimensions found in Ref. 15 can then be gleaned from the dipolar backflow analysis of a vacancy moving in an antiferromagnetic background.¹⁶ That is, the spin “twists” are generated by allowing for the mobile vacancy to minimize its energy. Such a state produces a non-zero quasiparticle weight, itself a requirement for a metallic phase.

Summarizing our results, we have completed the exact diagonalization for a 4×4 cluster with periodic boundary conditions for a binary alloy with a repulsive on-site Hubbard interaction. Our analysis has shown that the interactions generate an effective screening of the disorder potential for some fillings and disorder. Further, our real-space self-consistent Hartree-Fock (HF) solutions are seen to be able to reproduce quantitatively the local charge densities with considerable success, but not the quantitative details of the spin correlations. Our HF solutions display non-collinear, coplanar spin twists in the ground state at 1/2 filling when the disorder and interaction energies are comparable. This report will be followed by a longer paper with many more numerical results and detailed analysis.

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